

# A Multi-Scale Approach to Materials Model Development

ASC Materials & Physics Program

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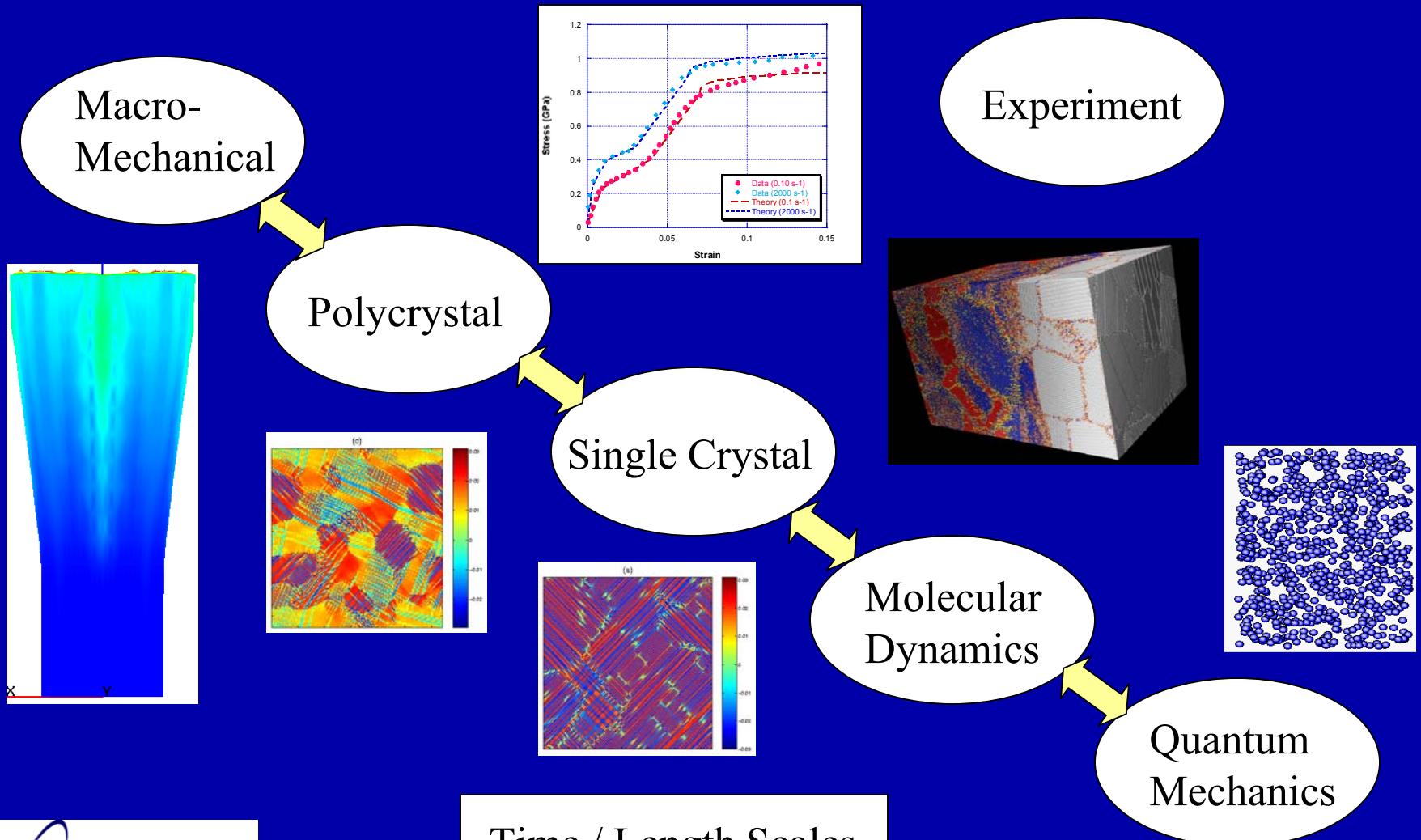
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Project Leader

LA-UR-03-2015



# Multi-Length Scale Approach

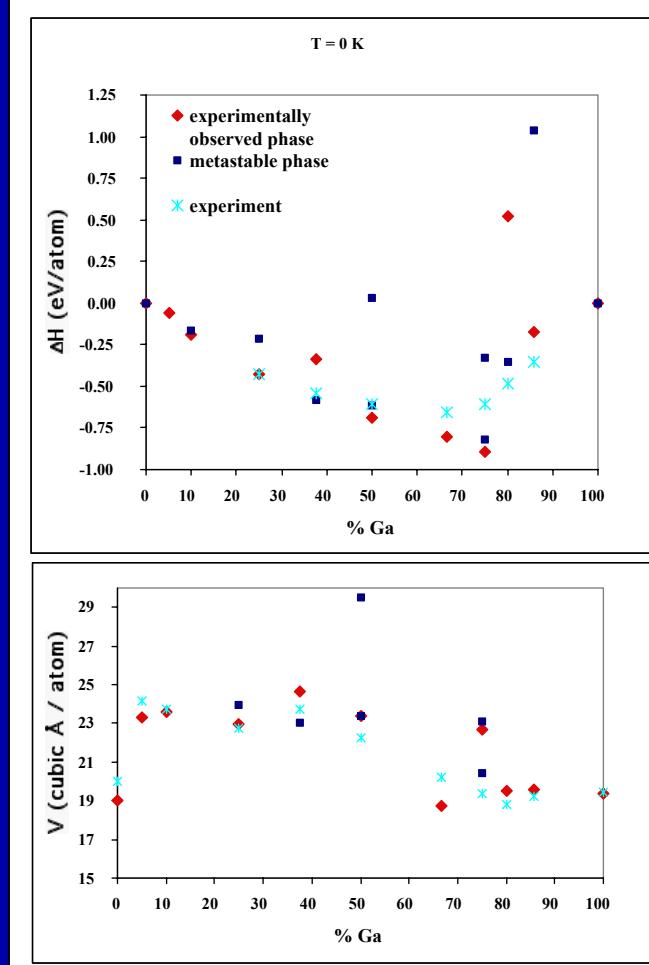


# Materials Effort Structure

- Atomistic Modeling of Metals (Albers)
- Organic Materials Modeling (Kober,Kress)
- Meso-mechanical Modeling (Albers,Preston)
- Macro-mechanical Modeling (Maudlin)
- Code Implementation (Maudlin)

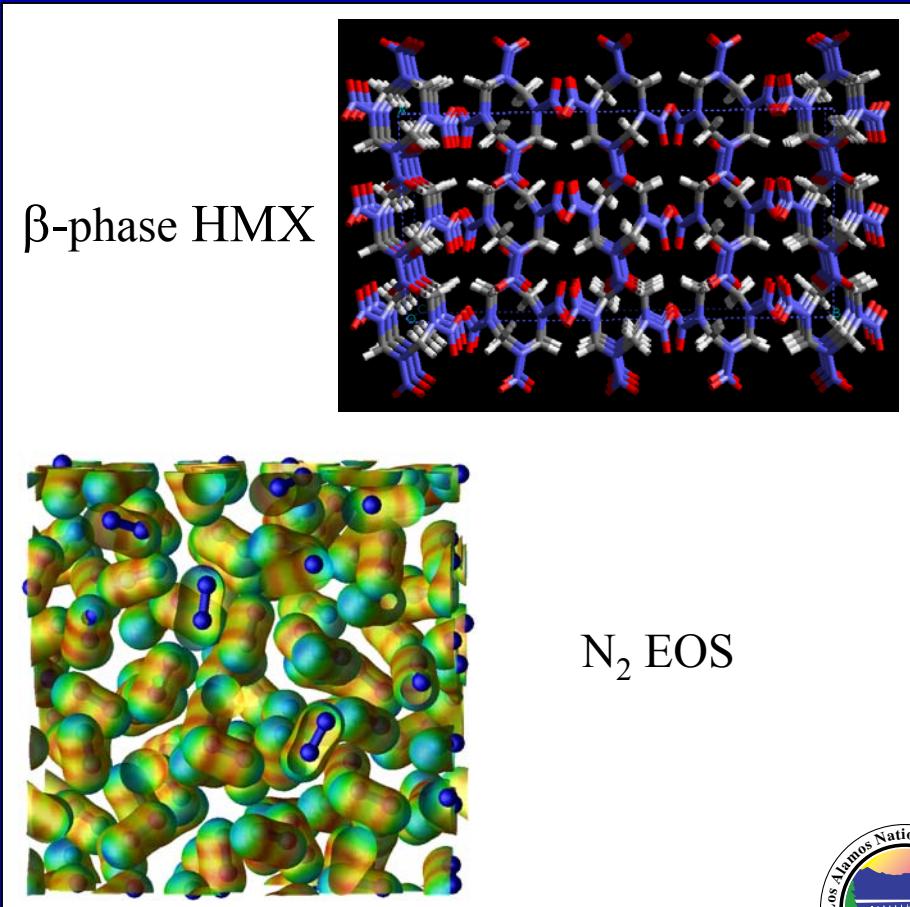
# Modified Embedded Atom Method (Baskes)

- Develop MEAM potentials
- Predict energy and volume of stable phases / compare to experiment
- Insight into Pu-Ga phase diagram
- Understand phase transf. under shock loading
- Aging effects on phase stability
- Implement potentials into MD simulations



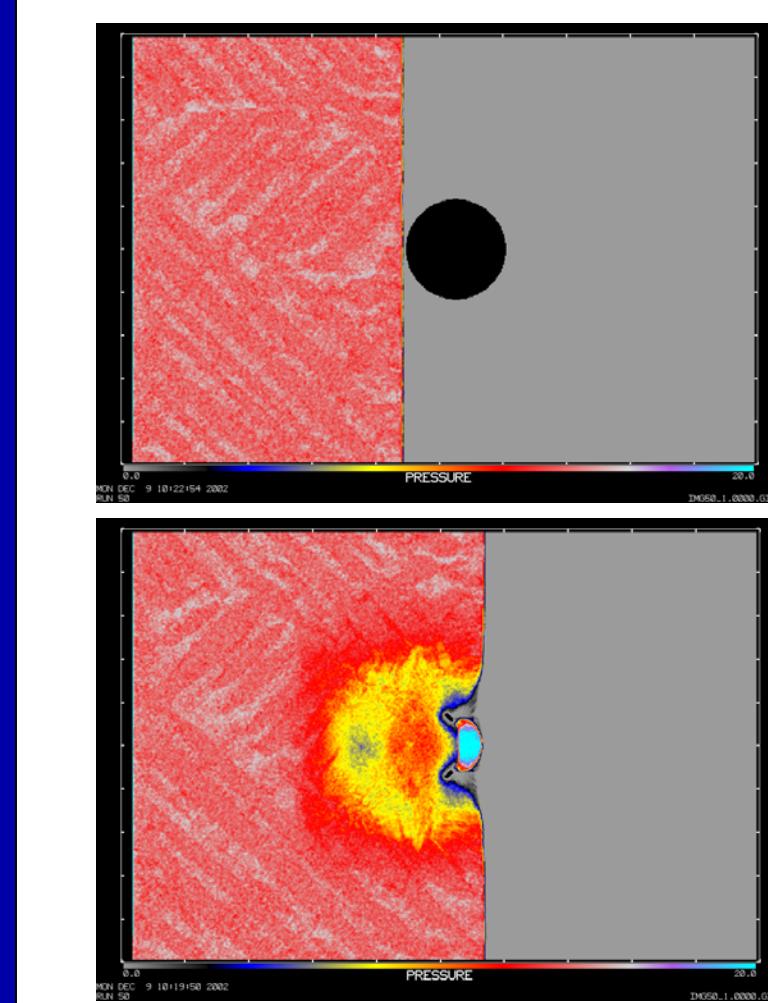
# Quantum Chemistry (Challacombe,Tymczak,Niklassen)

- Density Functional Theory
- Accurate forces / energies
- Three-dimensional, Periodic bndy. conditions
- Large scale ( $\sim 1000$  atoms)
- MondoSCF
  - Linear scaling
  - parallel



# Atomistic Molecular Dynamics (Germann, Lomdahl, Holian)

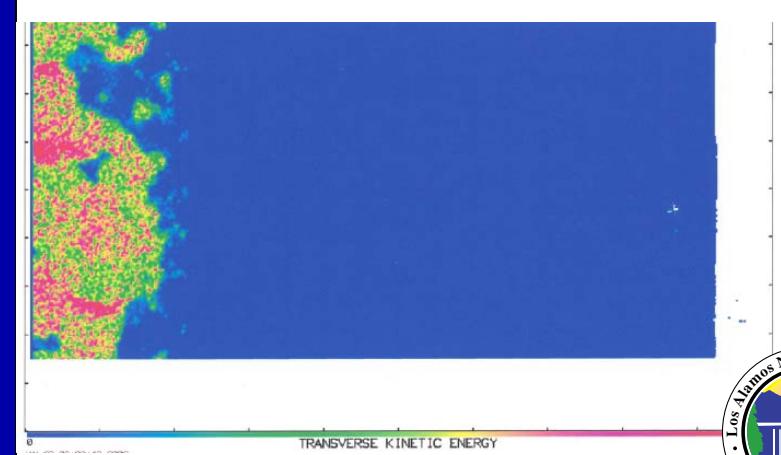
- SPaSM
- $10^9$  atoms
- Simple reactive potentials
- Polyatomic species
- Coarse-graining
- Applications
  - Strength
  - Detonation, ...
- Polycrystalline studies



# Polycrystalline AB Detonation

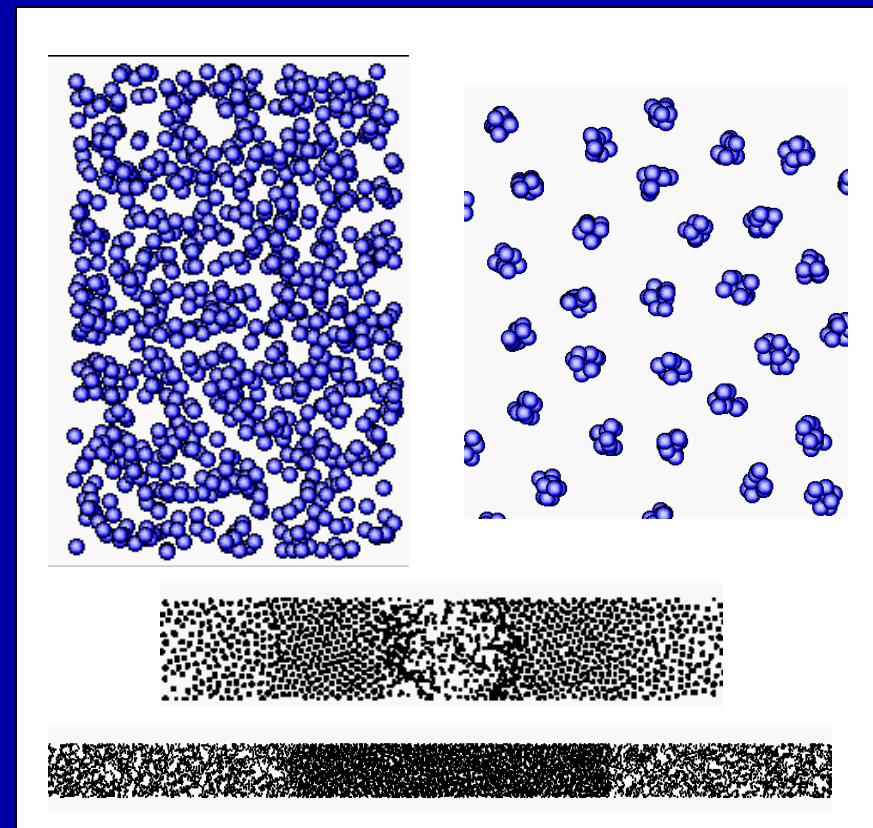
## (Germann, Lomdahl, Holian)

- SPaSM
- $10^8$  molecules
- Anisotropy and grain boundaries
- Material Strength
  - Elastic / plastic
  - Twinning
  - Molecules rotate
- Detonation



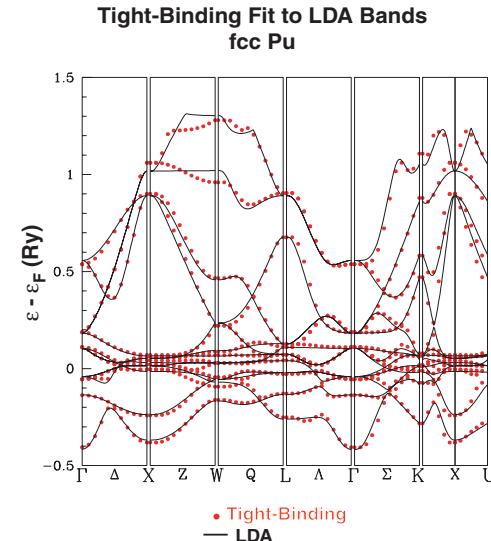
# Shocked Polymer Simulations (Valone)

- Novel atomistic model for polyethylene (MEAM)
- ~20 thousand atoms
- Decomposition
- Symmetric impact
- Crystalline sample shows two-wave structure, decomposition
- Amorphous sample shows one-wave structure
- Product analysis in progress

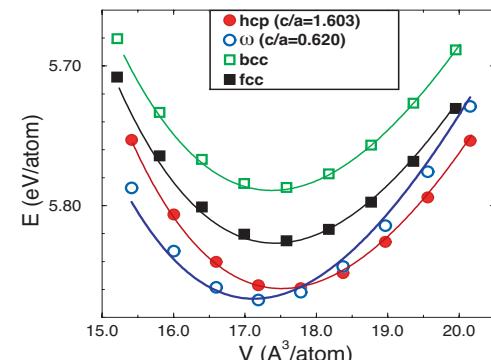


# Tight-Binding Atomistic Modeling (Albers)

- Atomistic materials models require high accuracy forces between atoms
- Tight-binding models:
  - Reproduce most accurate available 1<sup>st</sup> principles electronic structure calculations
  - Handle complex directional bonds of d- and f- electron materials (actinides)
  - Built in quantum mechanics
  - Allow extensions to finite temperature
  - Examination of complex structures (e.g. phase transformation paths, defects, grain boundaries, ...)

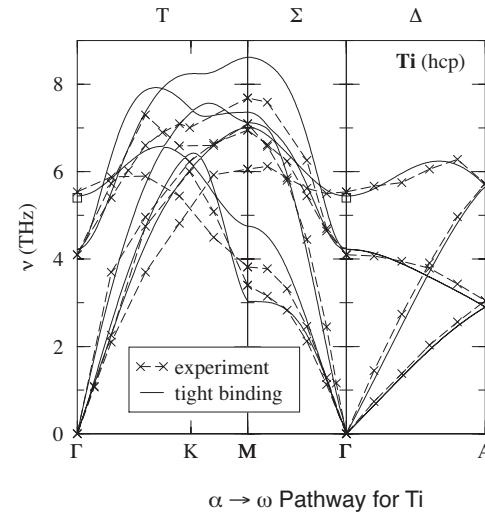


Titanium  
(comparison between tight-binding  
and 1st principles calculations)

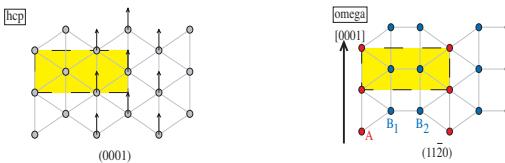


# Applications of Tight-Binding Methods (Albers)

- Applications of tight-binding methods:
  - EOS calculations
  - Phase stability and transformation paths
  - Phonons
  - Complex geometries (defects, grain boundaries, voids)
  - Diffusion barriers
  - Materials aging
  - Nonequilibrium materials properties
  - Mechanical properties

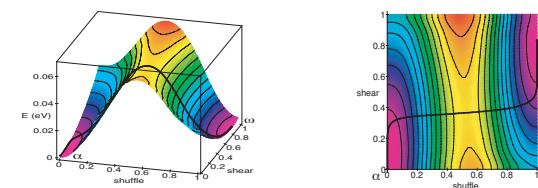


• Simple  $\alpha$  to  $\omega$  pathway (Silcock)



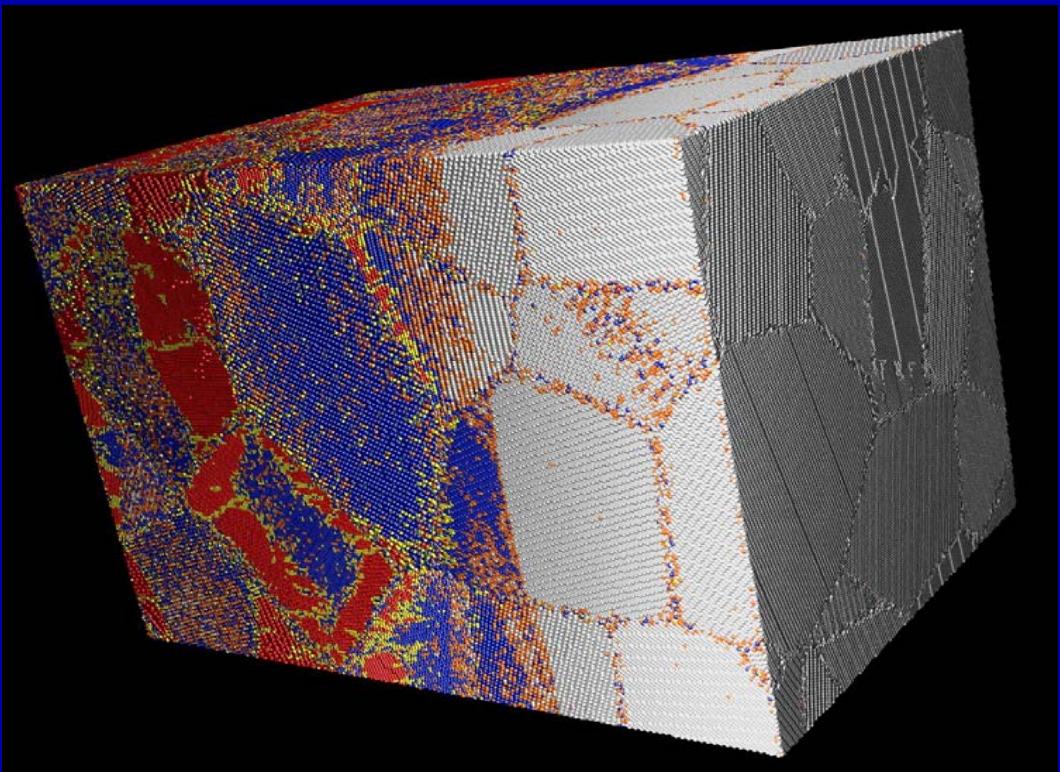
• We can study the pathway by assuming a homogeneous atom shuffle with unit cell shear.

$$E(\text{barrier}) = 49 \text{ meV}$$



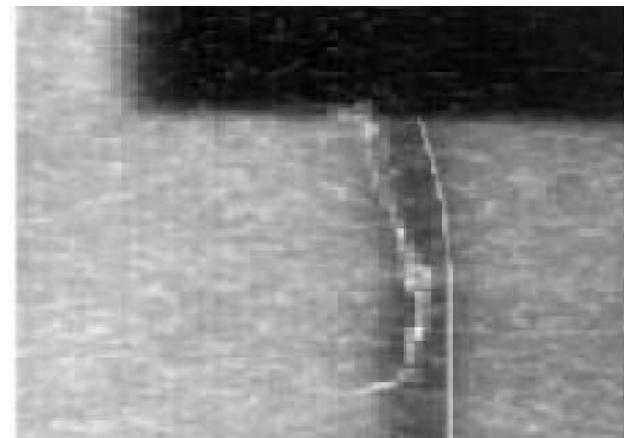
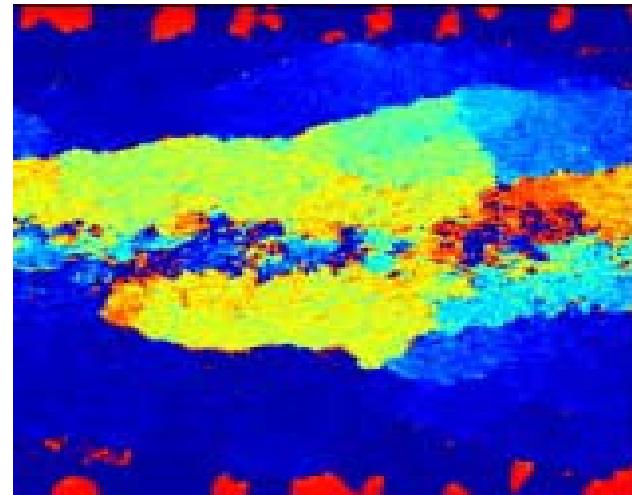
# Molecular Dynamics (Lomdahl, Holian, Germann, Kadau)

- Parallel Code
- Finite Range Pot.
- $10^8$  particles
- Time Scale  $10^{-11}$  s
- Length Scale 1 nm
- Shock Physics
- Phase Transf.
- Nano Crystals



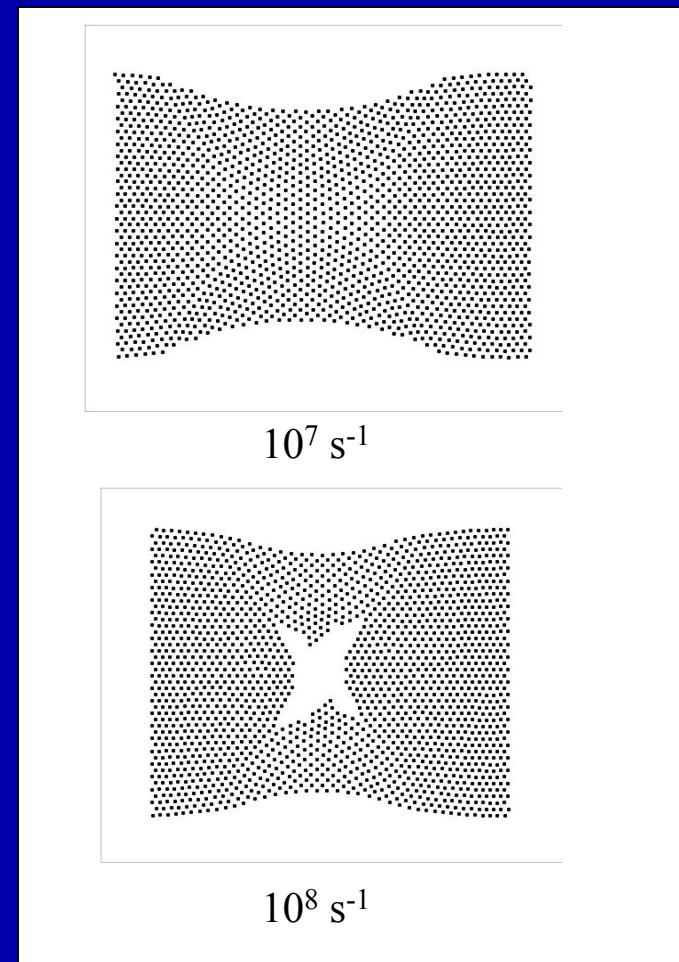
# Interfacial Dynamics (Hammerberg, Germann)

- Interfacial sliding
- Micro-simulations
  - NEMD
  - $10^5$  atoms
- Meso-simulations
- Comparison with experiment
- High shear velocities
- High pressure



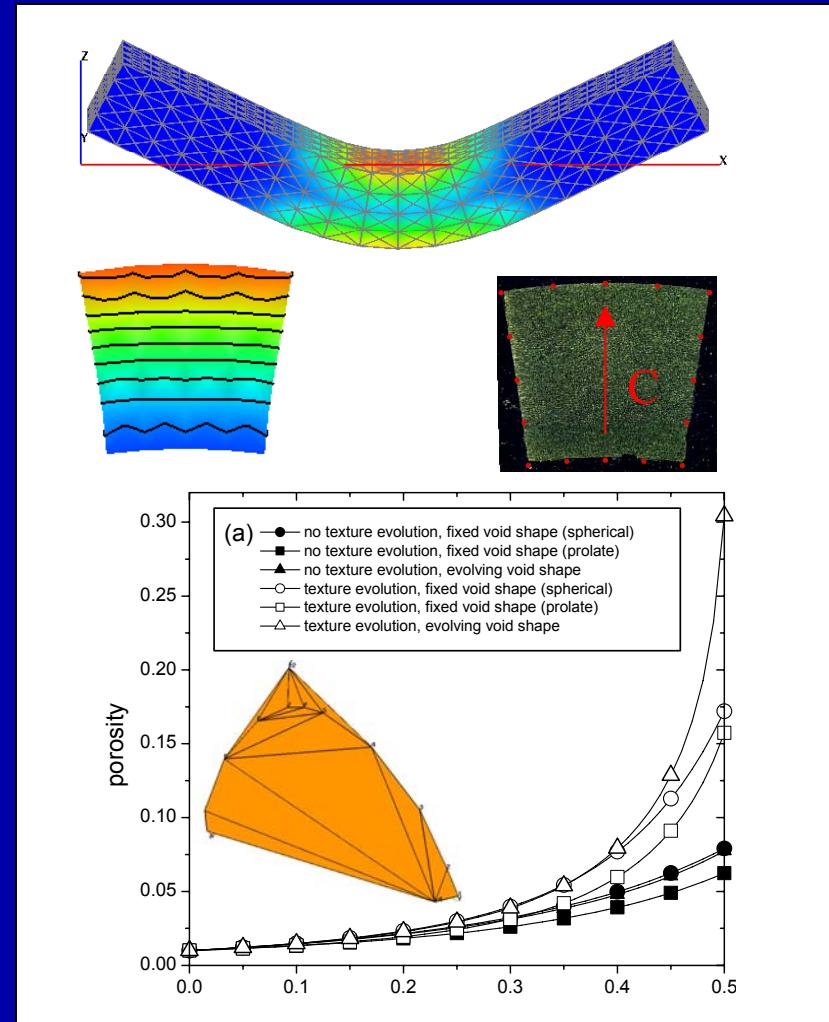
# Mesoscale Study of Ejecta and Spall (Reichhardt,Holian)

- New Effort
- Grain Size Particles (10nm)
- Simple grain potentials
- Add grain anisotropy
- Generalize approach
  - Parallelization
  - Improved potentials
  - Three-dimensions
- Program objectives:
  - Ejecta formation
  - Spall initiation



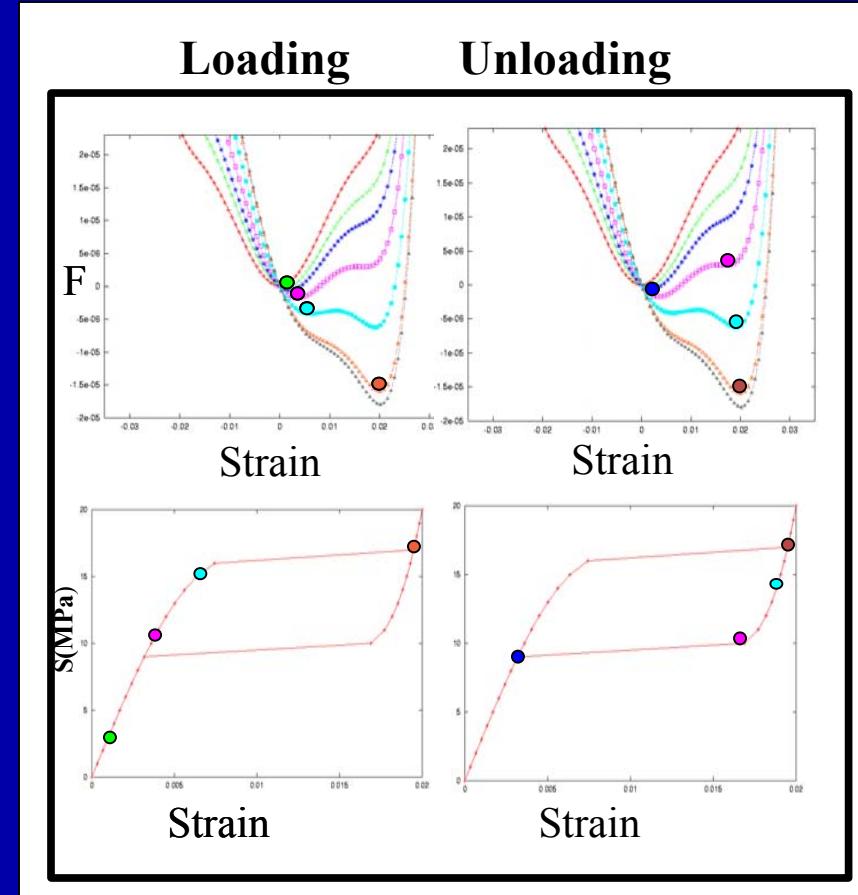
# Polycrystal Modeling (Tome, Kaschner, Maudlin)

- VPSC Model
  - Texture
  - Hardening
  - Damage
  - Twinning
- Response to Strain Path Changes
- Low Sym. Matls.
  - Be, Zr, Mg
- Exp'r. Support
- Coupled to FEA



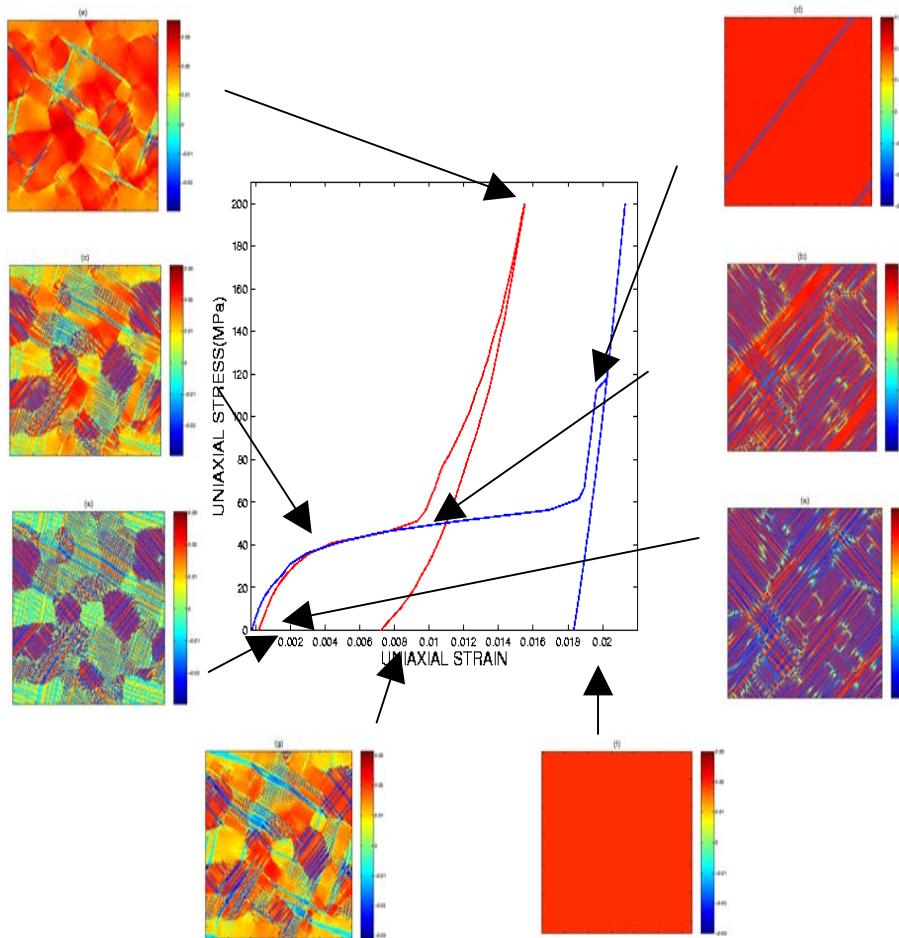
# Single Crystal Modeling (Saxena, Lookman)

- Ginzburg-Landau
- Phase Transf.
- Twinning
- Plasticity
- Stress / Strain
- Defects Nucleate
- Phase Transf.
- Polycrystal



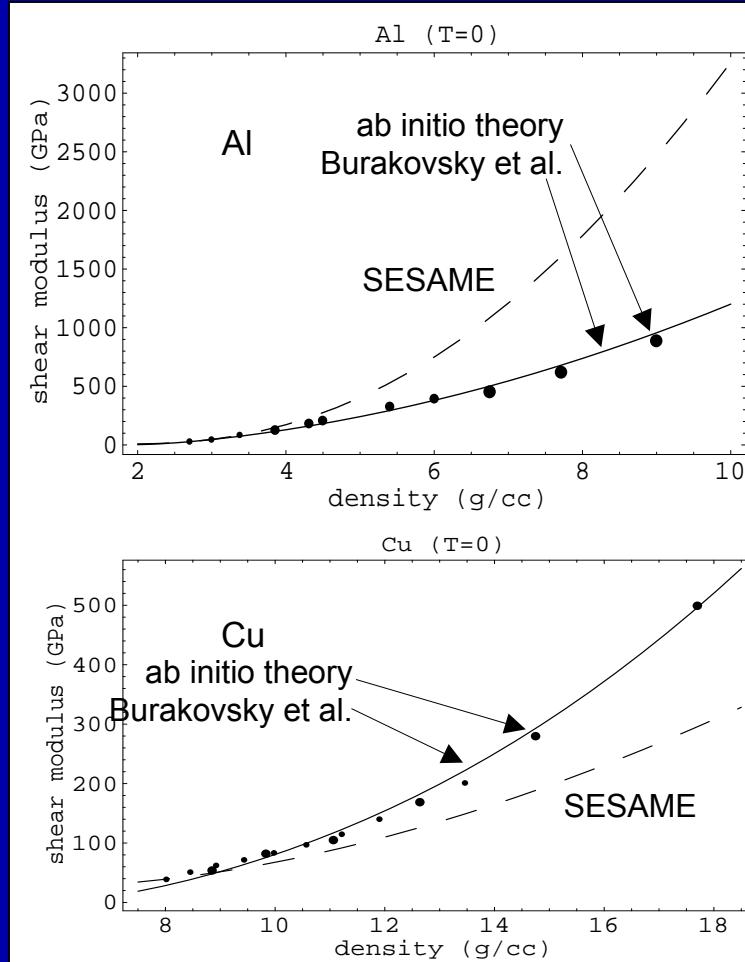
# Single Crystal Modeling (Saxena, Lookman)

## Loading and unloading of twinned martensite



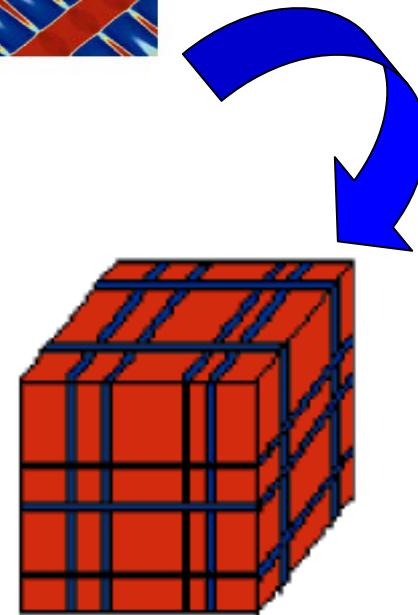
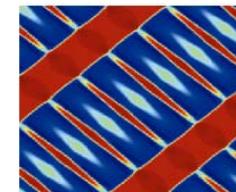
# Improved Material Properties (Burakovskiy, Preston)

- Shear Modulus (G)
- Gruneisen (G)
- Melt Curve ( $T_m$ )
- Wide  $\rho, T$  Range
- Shear Moduli added to SESAME
- Numerous (15) new unclassified tables



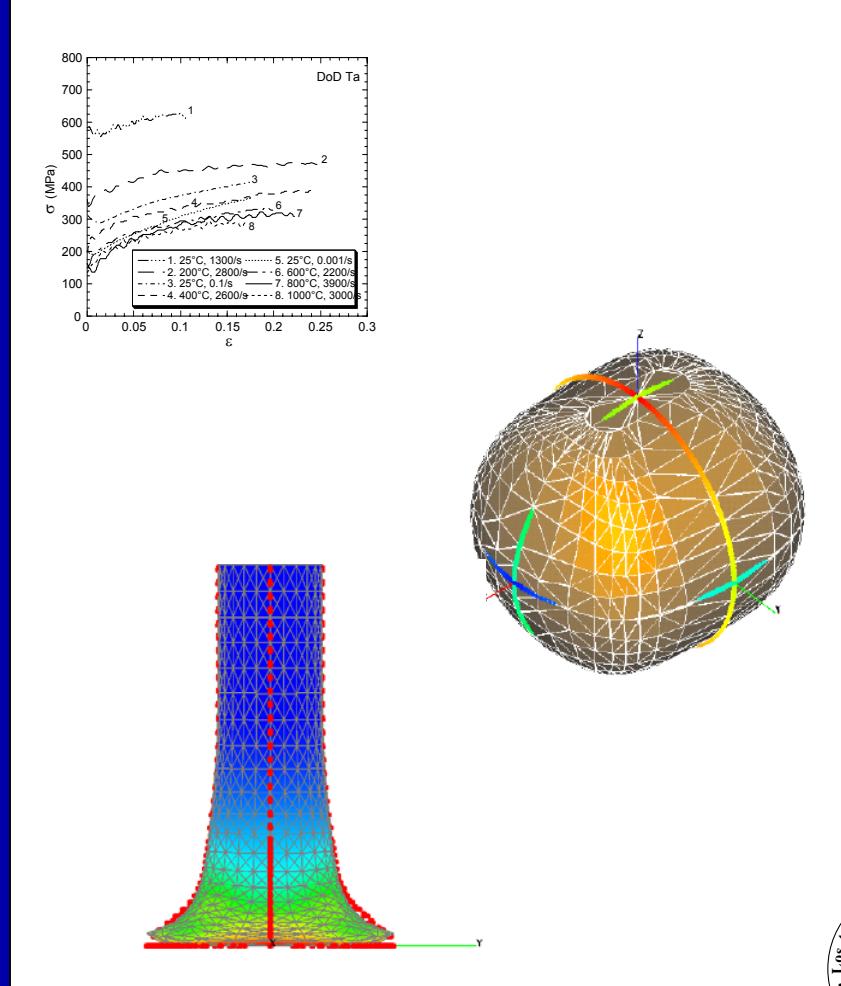
# Polycrystal Modeling (Lookman, Williams)

- Ginzberg-Landau Theory for Subcells
- Multivariant Theory for Subcells
- Gen. Meth. of Cells
- Phase Transformation
- Twinning
- Plasticity



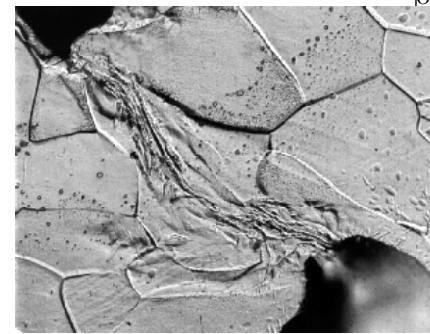
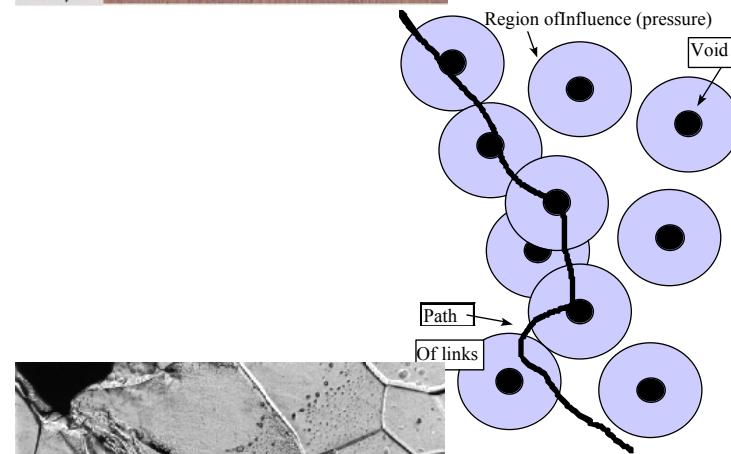
# Anisotropic Plasticity (Maudlin)

- Yield surface
  - $F(s_{ij}) - Y^2(\varepsilon, T, \dots) = 0$
- Rate-dependence
- Code implementation
  - EPIC, Antero
- Physically-based
- Exp'r. characterization
  - Texture
  - Flow stress
- Applied to numerous materials



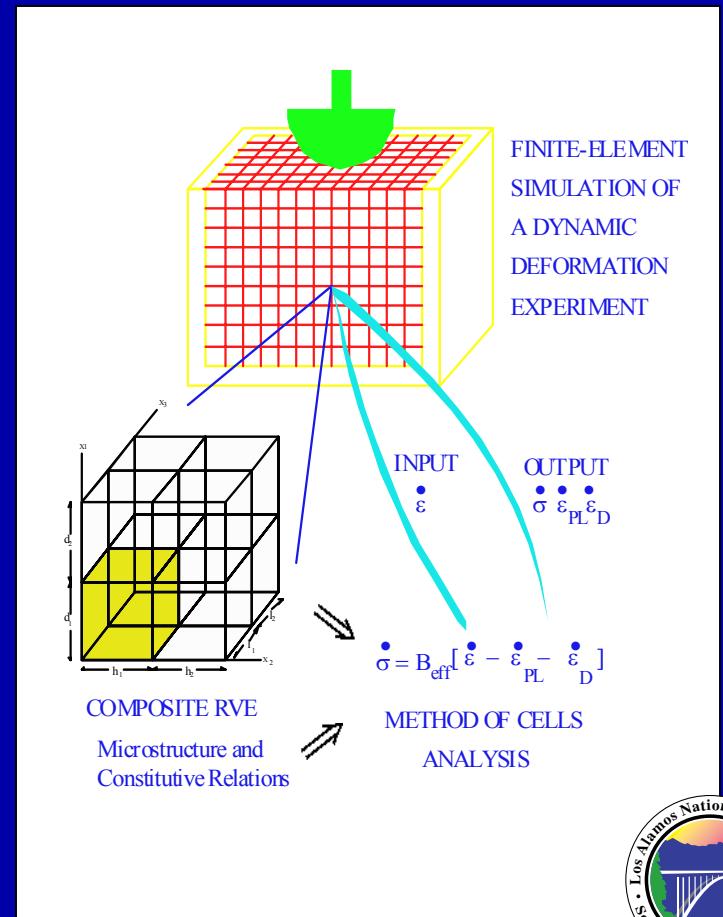
# Ductile Failure (Tonks)

- Rate-dependence/Inertia
  - Shielding / Void interactions
  - Void linking ranges
- Nucleation model
- Model development coupled to experiment
- General Failure Model
  - Shear and pressure
  - High- and low-strain rates
- Micromechanical Simulations
  - Analytical (isolated void)
  - Numerical (multiple void interactions)



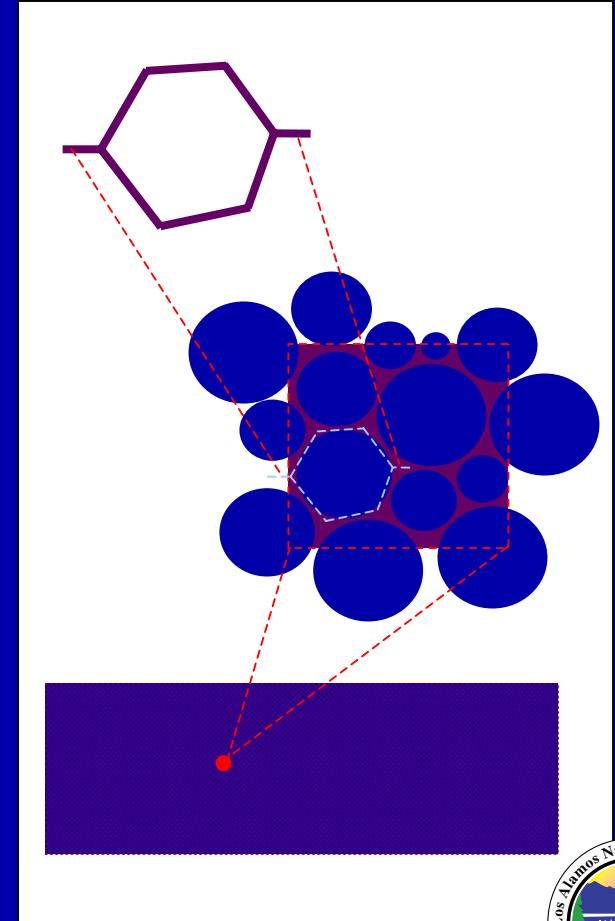
# Modeling Heterogeneous Materials (Addessio, Williams, Clements, Mas)

- Three-dimensional RVE
- Computational expense
- General constituent models
- Interface model
- Implemented in FEA
- Model Validation
- Numerous applications



# Modeling Foams (Schraad)

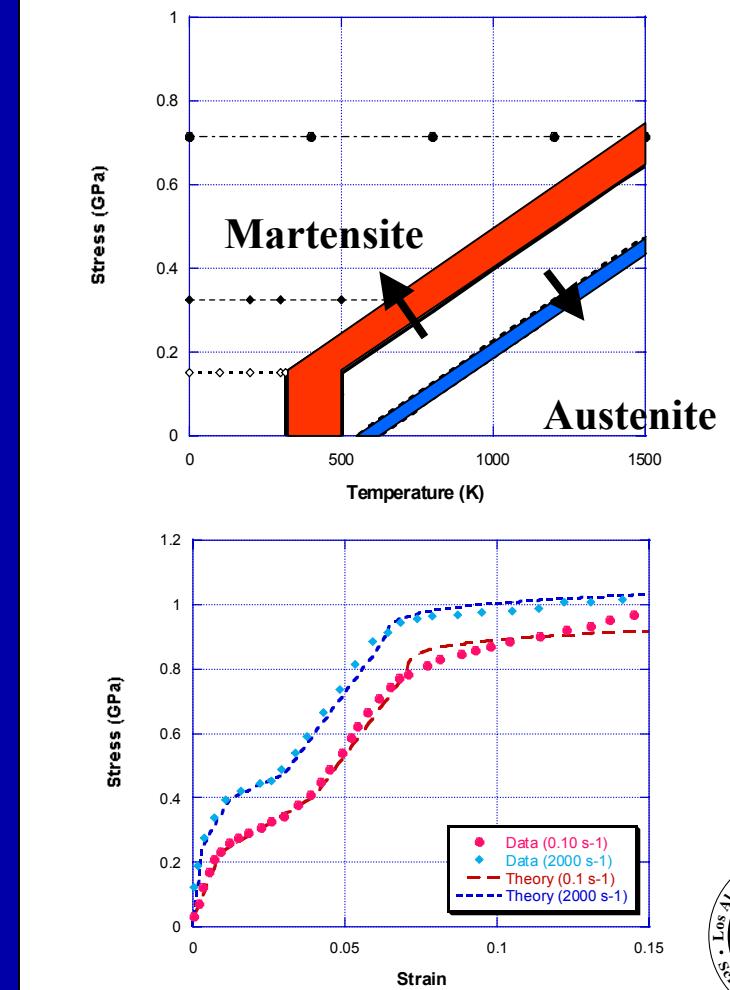
- Rate-dependent model
- Bridge cellular and global scales
- Valid for large strain, dynamic response
- Two-field approach
- PDF formulations



# Macro-Mechanical Model for U-6Nb

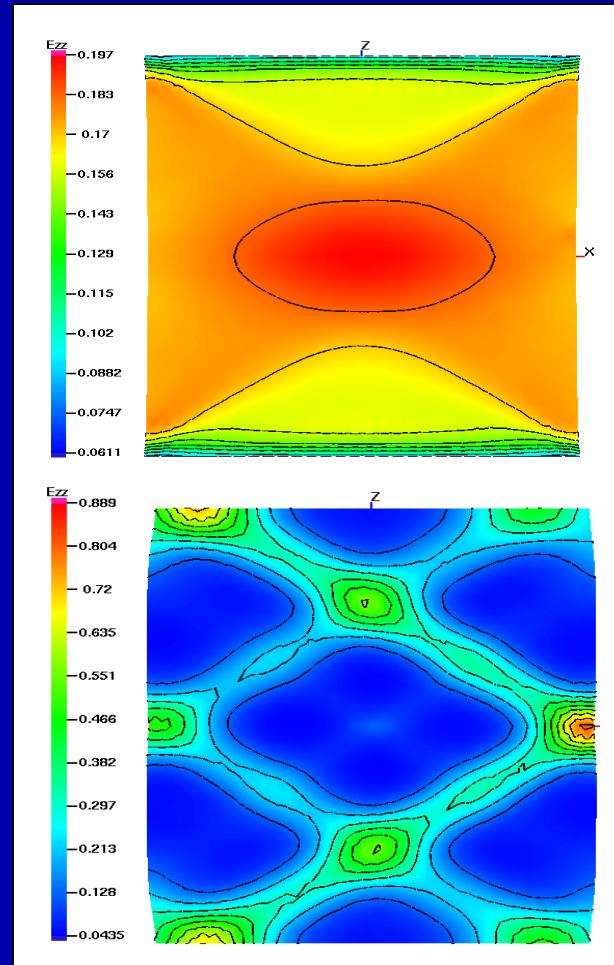
## (Addessio, Brinson, Mason, Zuo, Brown)

- Multiple Phenomena
  - Phase Transformation
  - Twinning
  - Plasticity
  - Ductile Failure
  - Equation of State
- Phase Diagram
- Isotropic Model
- Rate Dependence
- Implicit Numerical Tech.



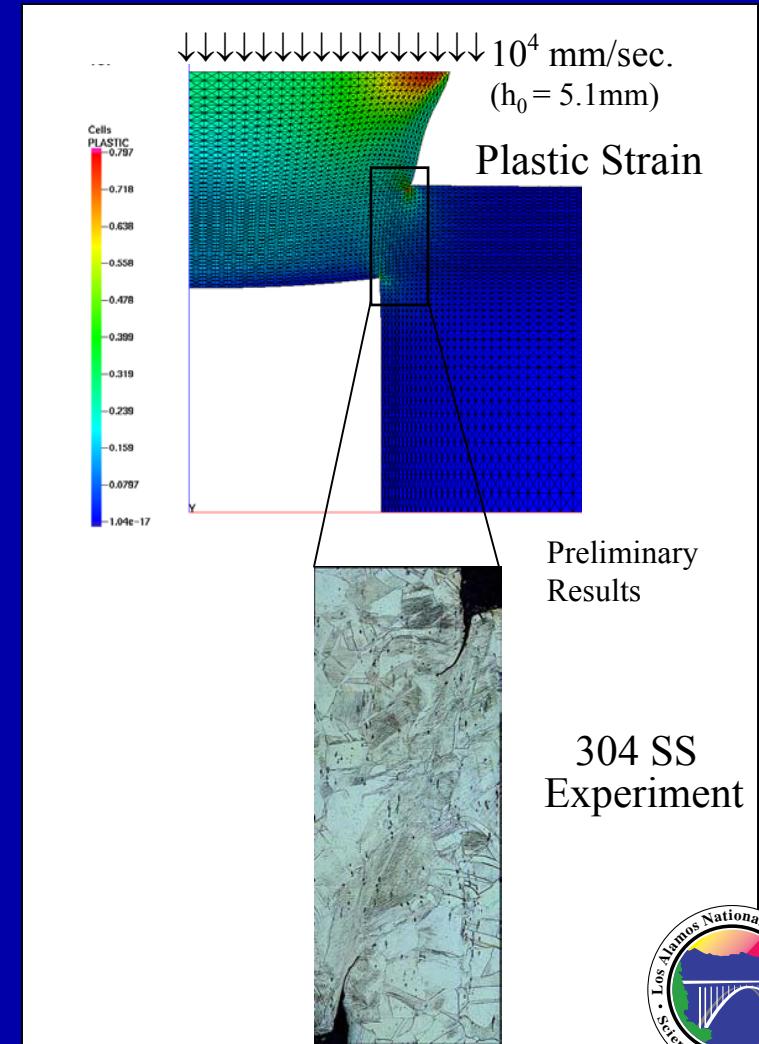
# Shear Localization (Maudlin, Zuo, Mason)

- Loss of Ellipticity
  - Time of failure
  - Direction of failure
- Comparison to Experiment
- Implementation into FEA
- Simulation of a Tensile Specimen (localization around an induced flaw)



# Modeling Shear Localization in Metals (Bronkhorst, Maudlin, Xue, Gray)

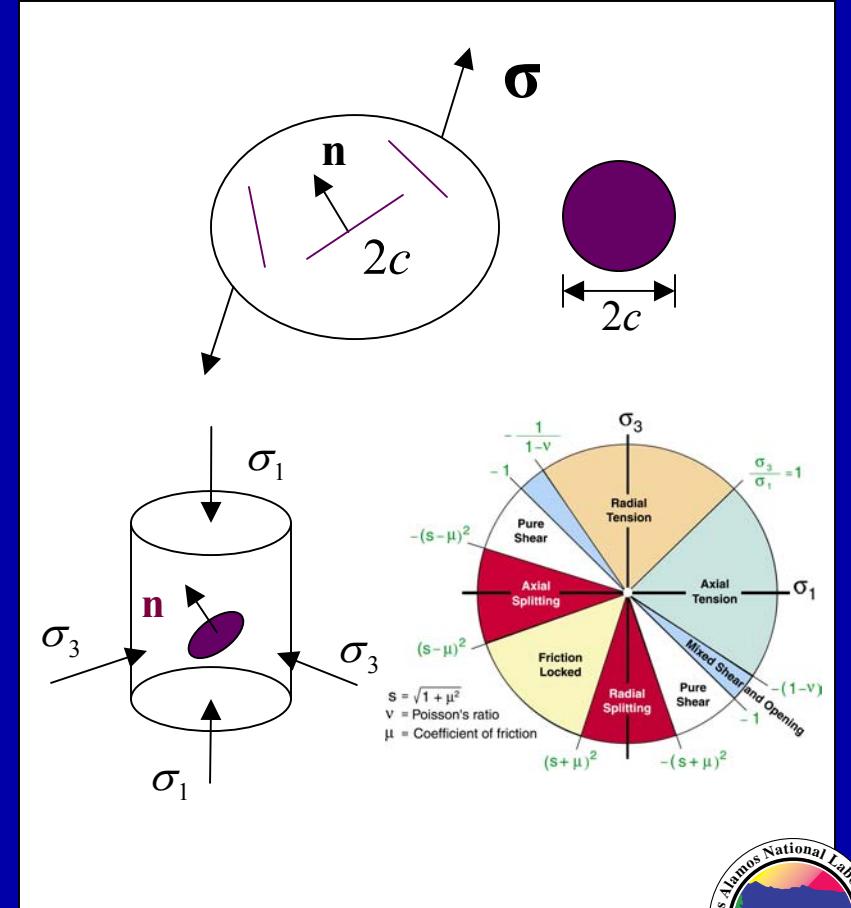
- Work has recently begun.
- Shear localization prominent in metallic ductile failure process.
- Localization not well characterized by material models.
- Deformation in experiment is complex.
- Numerical models necessary to understand experimental results.
- Modeling/Experimental work will lead to new material models.



# Modeling Damage in Brittle Materials

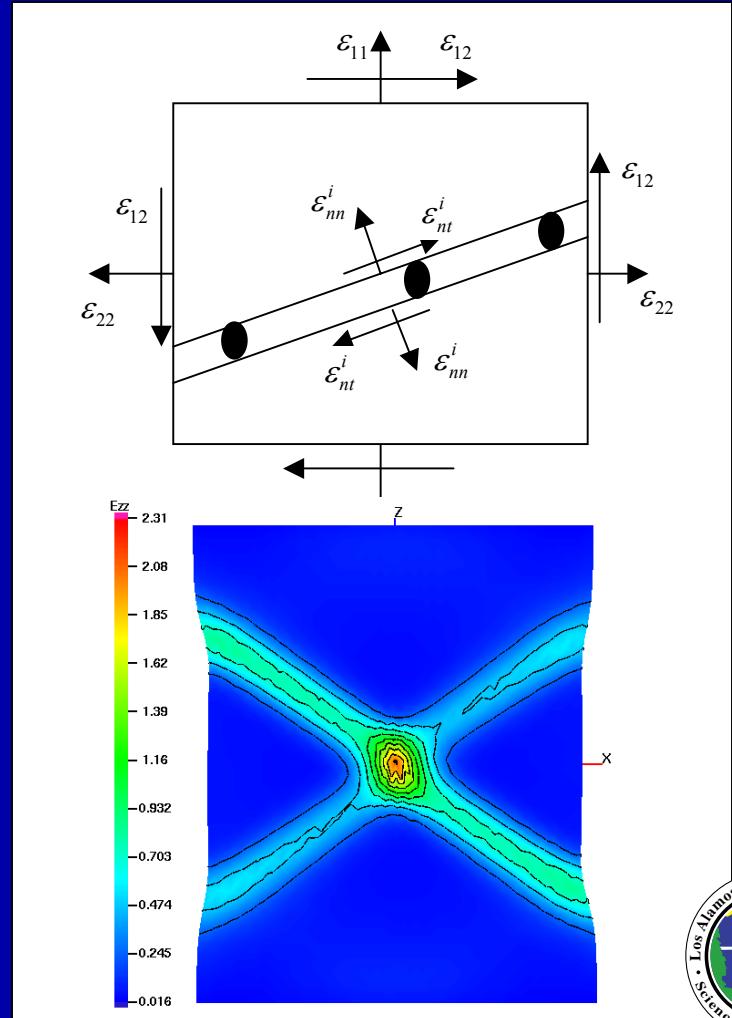
## (Zuo, Dienes, Maudlin)

- Simplified SCM
- Isotropic Model
- EPIC Implementation
- NWT Applications
  - Be
  - High-Explosives (HMX)
- Stability Analysis provides the Damage Surfaces



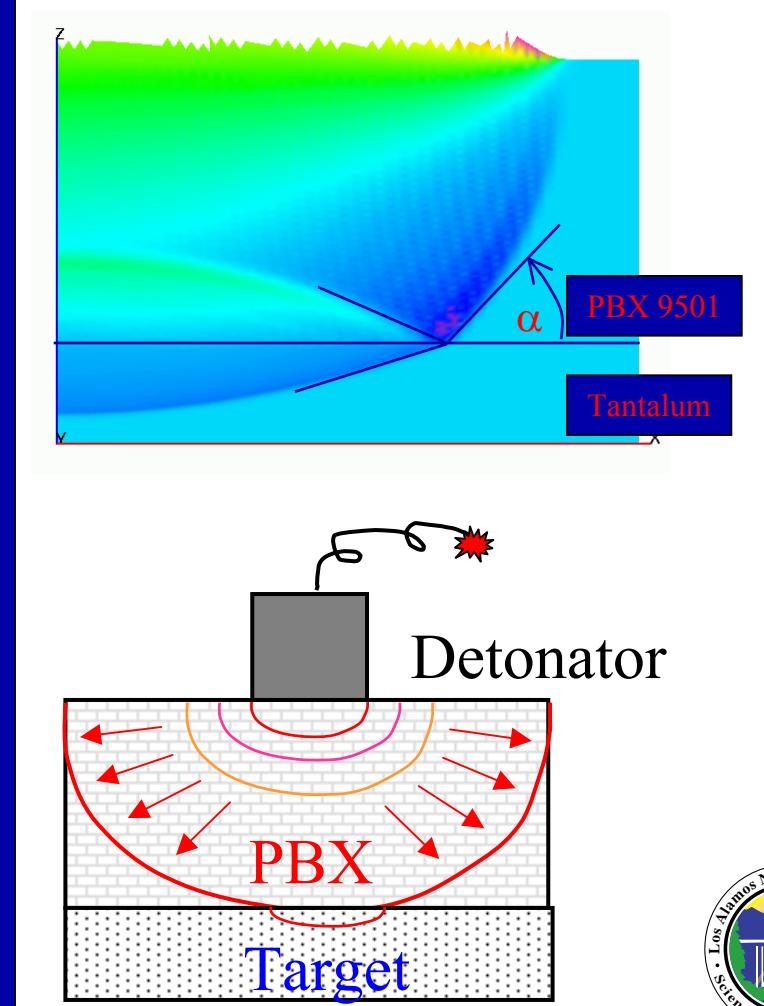
# Shear-Band Embedded Element (Zuo, Addessio, Maudlin)

- Shear Band Thickness (10  $\mu\text{m}$ )
- Engineering Analysis
- Composite Element
- Loss of Ellipticity
  - Instability
  - Direction
- Localization



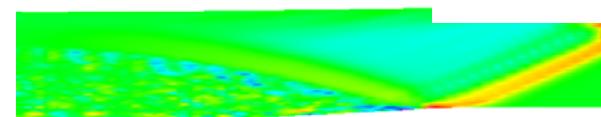
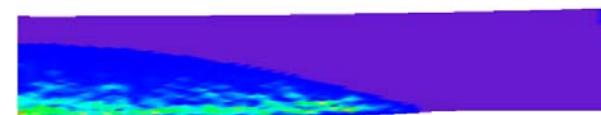
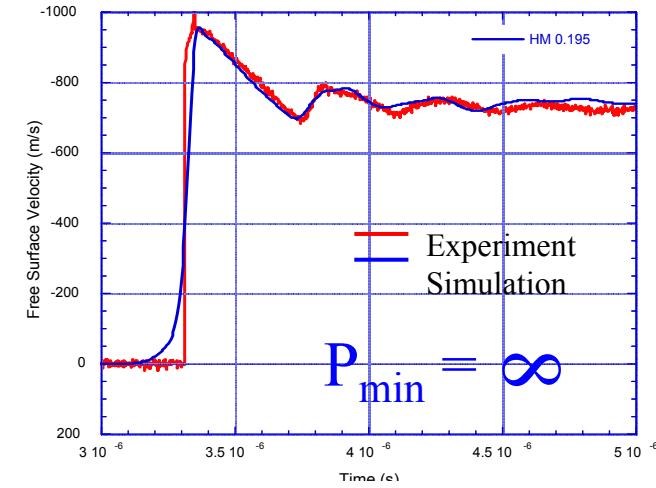
# Explosively Driven Shock Experiments (Mason, Maudlin)

- Exper. Diagnostics
  - PRAD
  - VISAR
- Simulations
- Materials
  - PBX 9501
  - Ta
- Shear Dominated



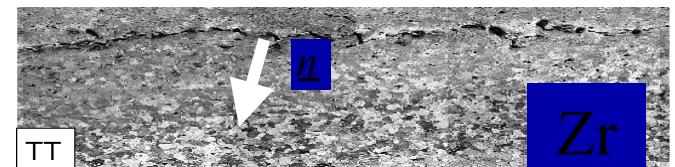
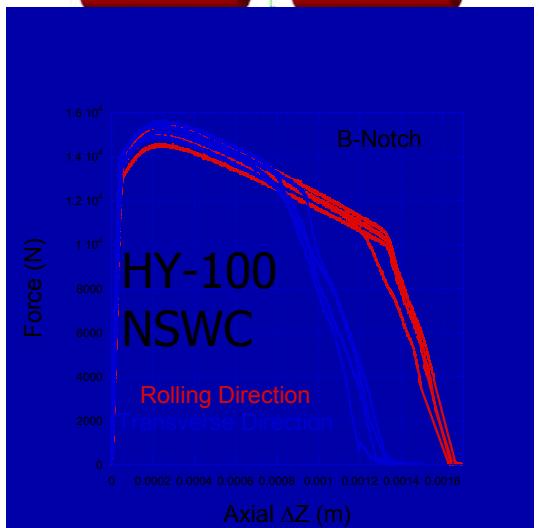
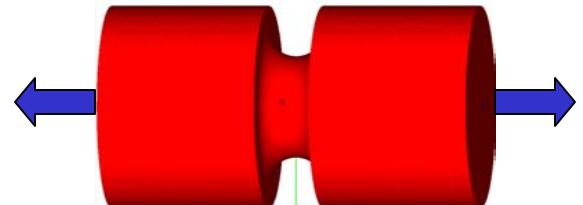
# Dynamic Fracture Modeling (Mason, Maudlin)

- TEPLA / EPIC
- Shear Dominated ( $P_{\min} = \text{large}$ )
- Post-Mortem characterization consistent with shear failure
- Interpretation of Data



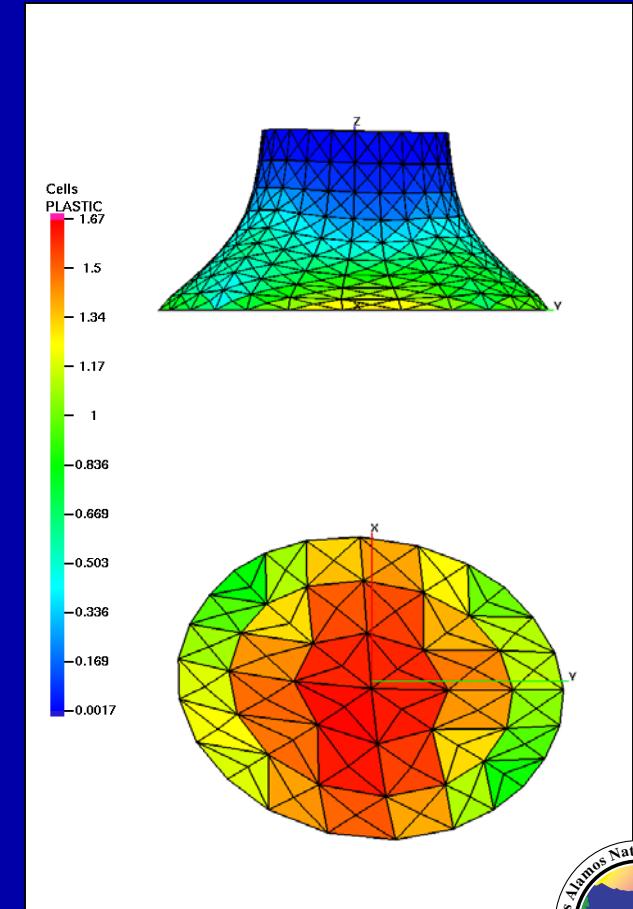
# Decohesion Model (Harstad, Maudlin)

- Predict Failure Direction and Rate
- Develop Isotropic Decohesion Model
- Comparison to HY-100 Notched Bar Data
- Capture Failure by Void Sheeting
- Extend to Anisotropic Model (elliptical voids / failure)



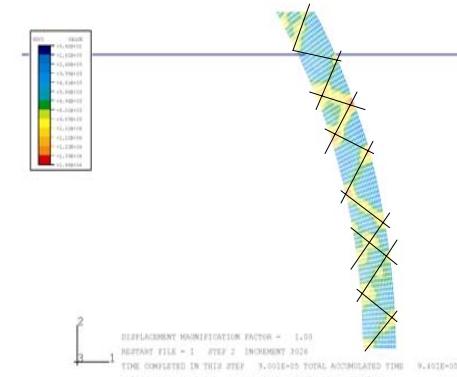
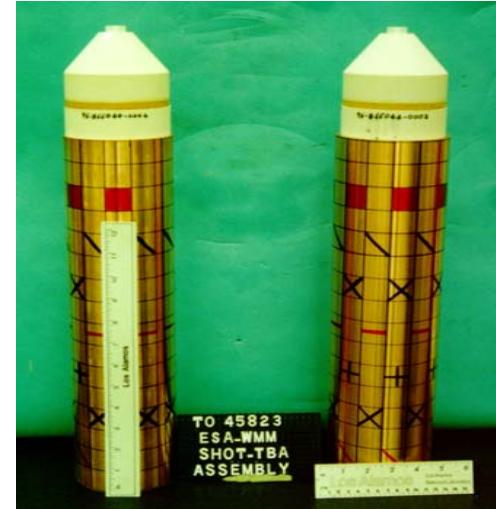
# Code Implementation (Harstad)

- Numerically Robust
- Computationally Efficient
- Anisotropic Elasticity
- Anisotropic Plasticity
- Ductile Failure
- Suite of Validation Probs.
  - Plate Impact
  - Taylor Impact
  - Uniaxial Stress
  - Low- / High- Strain Rate



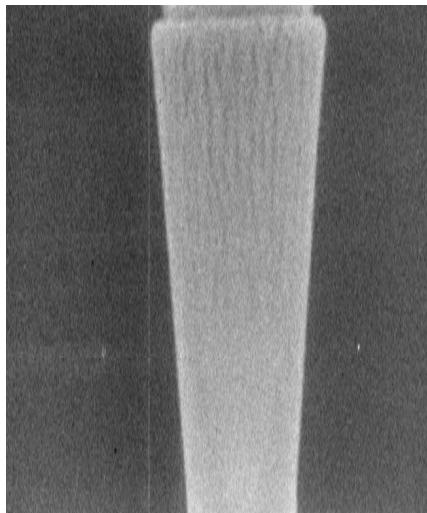
# Code Implementation (Zocher, Prime, Canfield)

- Models Implemented into ASCI & Materials Codes
  - Shavano Project
  - Antero Project
  - Blanca Project
  - EPIC
  - DYNA
- Assist in Code Debugging
- Code Milestones
- Interactions on General Materials Package
- (Prefer Lagrangian / ALE)
- (Prefer Stable Codes)



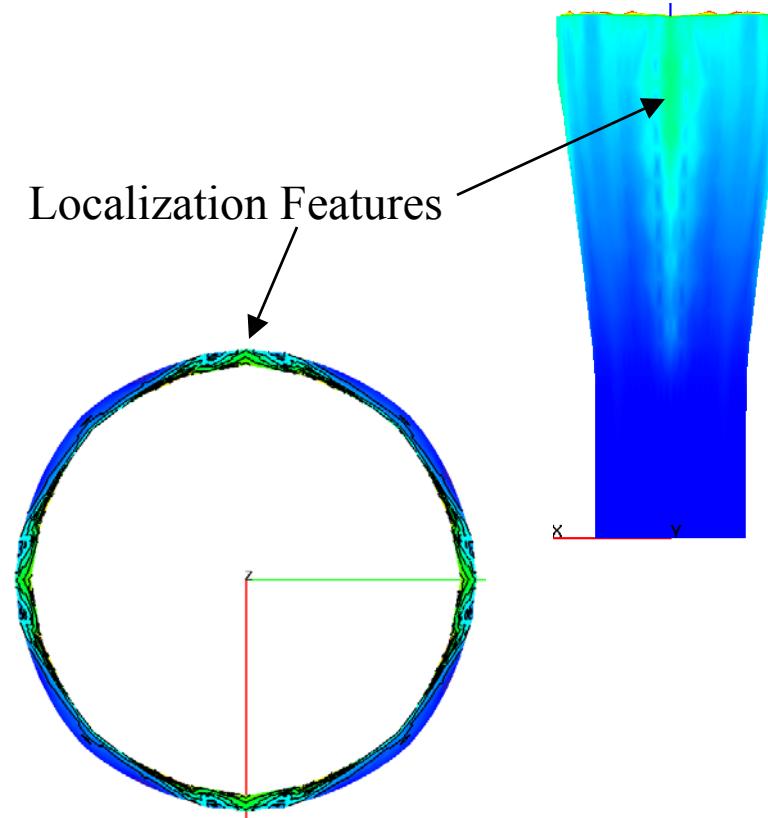
# Expanding Cylinder Simulations (Maudlin, Zuo, Mason)

Test Radiograph



Three-dimensional simulations  
(plastic strain contours)

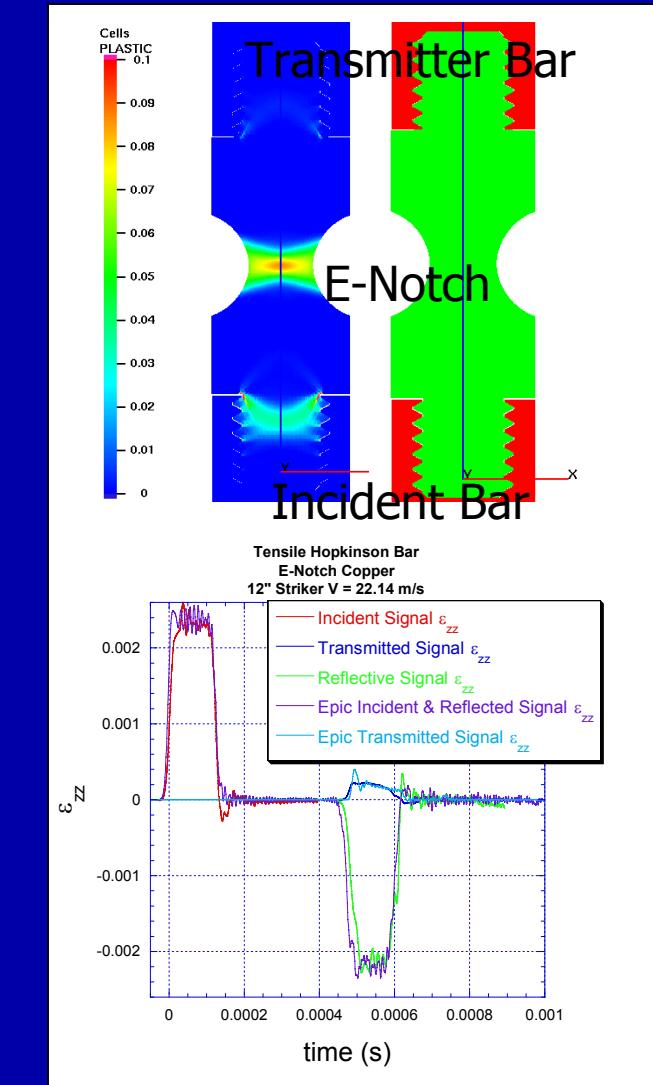
Localization Features



Los Alamos

# Model Validation

- Low-/High-Strain Rate
- Tensile / Compr. Hop. Bar
- Taylor Impact
- Plate Impact
- Four Point Beam
- Notched Bar



# Summary

- Multiple Length Scale Approach
- Coupled to Experimental Efforts
- Code Implementation of Models
- Multi-Divisional Effort
- Scientific Quality
- Highly Leveraged Effort (MOU)
- Issues:
  - Experimental Data
  - Stable Codes

